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Data needs for stellar atmosphere and spectrum modeling

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ABSTRACT

The main data need for stellar atmosphere and spectrum modeling remains atomic and molecular transition data, particularly energy levels and transition cross-sections. We emphasize that data is needed for bound-free ($b-f$) as well as bound-bound ($b-b$), and *collisional* as well as radiative transitions. Data is now needed for polyatomic molecules as well as atoms, ions, and diatomic molecules. In addition, data for the formation of, and extinction due to, liquid and solid phase dust grains is needed. A prioritization of species and data types is presented, and gives emphasis to Fe group elements, and elements important for the investigation of nucleosynthesis and Galactic chemical evolution, such as the α-elements and n-capture elements. Special data needs for topical problems in the modeling of cool stars and brown dwarfs are described.

1. Introduction

It has long been known that the radiative extinction of gas plays a major role in determining both the structure of a stellar atmosphere and the emergent spectral energy distribution. Accurate knowledge of the extinction requires accurate knowledge of transition wavelengths, λ, and of transition cross sections, σ_ν (or, equivalently, for bound-bound ($b-b$) transitions, oscillator strengths (gf values)), which in turn requires accurate knowledge of the energy level (E-level) structure of atoms, ions, and molecules. With the discovery and classification of an increasing number of brown dwarfs, for which atmospheric temperatures are lower than that of the coolest objects that are traditionally regarded as stars, there is now a need for molecular data for polyatomic molecules, in addition to that for diatomic molecules (Allard *et al.* 2003).

The importance of the $b - b$ transitions, which give rise to spectral lines, has been well documented. However, bound-free ($b - f$) transitions also significantly determine the atmospheric structure and spectral energy distribution of stars, and accurate knowledge of the corresponding cross-sections, σ_ν, is crucial. The importance of radiative transitions has been long recognized because they contribute directly to extinction. However, for realistic treatments, collisional transitions also play a central role in determining the equilibrium state of the gas, and thus, through the physics of radiative transfer, the emergent spectrum.

As a point of general motivation, we note that there is a long tradition, still being practiced, in quantitative stellar spectroscopy of "tuning" atomic parameters so that solar atmospheric models match solar spectral features of interest. This approach is based on the assumption that we have a correct model of the solar atmospheric structure and correct solar abundances. Therefore, it is particularly disconcerting to note that the solar abundances of C, N, and O have recently been revised downward by factors of two to three on the basis of including turbulent hydrodynamic structure in the atmospheric model (Asplund 2000). Furthermore, the solar abundance of Fe is still in dispute by a factor of 1.5 (Kostik *et al.* 1996). Clearly, it would be helpful to remove the atomic data as a "variable" from this process.

In addition to atomic and molecular data, extinction cross sections for liquid and crystalline aerosols of all types are needed. Again, it is in the cool brown dwarf objects that aerosols play a significant role in the atmospheric structure and emergent spectrum (Allard *et al.* 2003).

2. Atomic data

2.1. Prioritization

One way to rank the chemical elements in urgency is to weight them by the product of their relative abundance in stellar atmospheres and the richness of the line spectrum that they contribute. With this ranking, iron (Fe) and the Fe group elements have the highest priority. Another prioritization is to weight the elements by their importance to particular problems in nucleosynthesis and Galactic chemical evolution. By this criterion, the α-process and neutron capture (n-capture) elements deserve urgent consideration.

2.2. Fe group

Fig. 1 shows the E-level diagrams for atomic models of Fe I and II that are based on laboratory and semi-empirical atomic data of Kurucz (1994) and Kurucz & Bell (1995). From

the energy gap between the highest included bound E-levels and the ionization limit, we conclude that the atomic models are not complete. In addition to the E-levels and transitions displayed in Fig. 1, Kurucz (1992) has also made available data for hundreds of levels and thousands of lines on the basis of theoretical quantum mechanical calculations. Kurucz (1992) has demonstrated that inclusion of these additional theoretical lines in solar atmospheric modeling reduces the predicted solar flux in the UV band, thus allowing theoretical solar atmospheric models to fit the observed UV band flux much more closely than was previously possible. However, when high resolution synthetic spectra computed with the theoretical lines are compared to the observed solar spectrum, the match is *worse* than when the theoretical lines are omitted from the calculation (Bell *et al.* (1996), Short & Lester (1996)). This is due to the pervasiveness of significant errors in the E-level values (and, hence, transition λ values) and in the gf values. It should be noted that Kurucz (1992) himself acknowledged at the outset that the theoretical lines should only be used for stellar atmospheric structure and broad-band flux level calculations. This points to the need for more reliable and complete measurements of E-levels and gf values for Fe.

Need for completeness: It is worth noting that although many of the Fe transitions seen in Fig. 1 give rise to very weak lines, it has been long understood that thousands of weak lines of a particular element concentrated in a particular band, such as the near UV, act collectively as a broad-band pseudo-continuous veiling opacity that can significantly affect the atmospheric structure and the emergent flux level (the "iron curtain" effect) (Rutten 1986). Furthermore, in non-local thermodynamic equilibrium calculations (non-LTE), high lying E-levels can act as an important channel of ionization to the ground state of the next higher stage, and their neglect in the atomic model can lead to erroneous results for the ionization equilibrium (see, for example, Short & Hauschildt (2005)).

There is a particular dearth of atomic data for Fe ionization stages greater than II, especially for $b - b$ transitions of $\lambda < 2000$ Å (ie. vacuum UV and far UV (FUV) band transitions). Stages III and IV, and UV transitions thereof, are important for the study of hot stars (spectral class O and B), and the chromospheres and transition regions between the chromospheres and coronae, of solar type and relatively cool stars. Stages XII through XIV are useful for modeling the X-ray band spectra of stellar coronae.

LS coupling: Another area of concern is the lack of atomic data from quantum mechanical calculations for transitions that are not predicted under the assumption of LS coupling. For example, Fe III has been detected outside the H II regions around hot stars, yet of the 64 terms of Fe II, as predicted by LS coupling, none have transitions to Fe III of $\lambda < 911$ where photo-ionizing flux may escape from the H II region. This indicates that non-LS coupling transitions may be important, and the data for them should be measured.

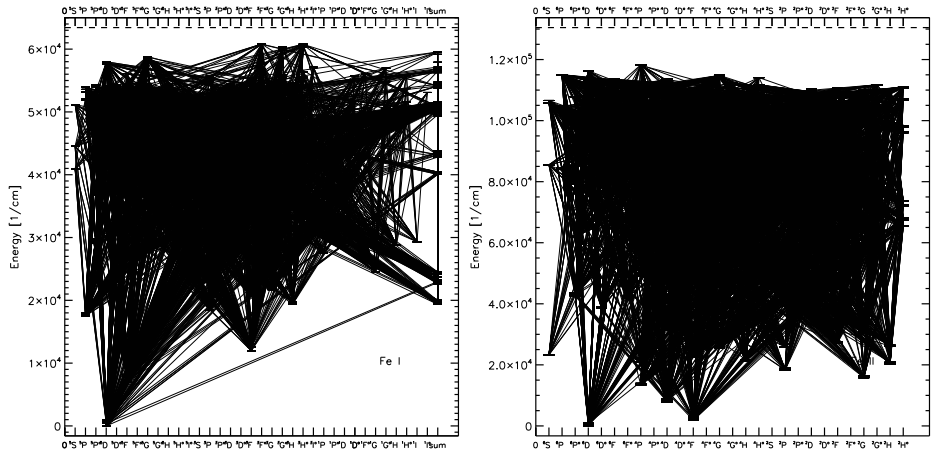

Fig. 1.— Grotrian diagrams of the models of Fe I (left) and II (right) based on the laboratory and semi-empirical data compiled by Kurucz (1994) and Kurucz & Bell (1995).

2.3. Nucleosynthesis and Galactic chemical evolution

α-process elements: There is a particularly urgent need for improved data, or any data at all, for the following elements associated with He fusion and the α-process: 1) gf values for $b - b$ transitions of Mg I and Si II; 2) σ_ν values for $b - f$ transitions of C I and II, Mg I and II, and Ca I and II; 3) low E (0-5 eV) e^- and H collisional σ_ν values for O I, Mg I, Al I, and Ca I.

n-capture elements: The advent of 8-m class telescopes has allowed the acquisition of spectra of faint Galactic halo red giant stars of sufficient quality to allow quantitative analysis. This includes the extremely metal poor (XMP) stars, in which $[\frac{\mathrm{Fe}}{\mathrm{H}}]$ is less than -3, and can be as low as -5. In these stars, the "iron curtain" referred to in Section 2 is relatively transparent. As a result, investigators have detected spectral lines of relatively heavy elements that are formed by the n-capture process (both the rapid (r-process) and slow (s-process)). The spectroscopic determination of the abundances of these elements is important for the investigation of the astrophysical sites of nucleosynthesis, the formation of the Galaxy, and the nature of the first stars. However, quantitative analysis will require accurate and complete atomic data of the sort that has been long called for in traditional light element analysis.

2.4. General atomic considerations

Bound-bound transitions: Given the constraints on measuring (or calculating) atomic parameters, there has been a tendency for stellar spectroscopists to prioritize by emphasiz-

ing those transitions that give rise to spectral lines that are useful abundance diagnostics. However, we note that extinction due to *all* transitions contributes to determining the radiative equilibrium (RE) structure of a stellar atmosphere. Furthermore, in non-LTE modeling determination of the excitation and ionization equilibria is a non-local problem such that the rate of *any* transition may affect the rate of any other (multi-level non-LTE effects). Worse, to the extent that different chemical species may have transitions that overlap in wavelength, the computed strength of a spectral line of one chemical species may depend on the equilibrium state of other species (multi-*species* non-LTE effects) (see Short & Hauschildt (2006) for examples of the non-LTE effect of Fe group elements on Sr and Ba lines). Therefore, accurate modeling of any spectral feature can depend on accurate atomic data for many transitions, not just the transition that directly corresponds to that spectral feature.

Bound-free transitions: Bound-bound transitions receive much attention because of the obvious importance of spectral lines. However, photo-ionization and recombination rates are also of central importance to calculating the equilibrium state of a gas and radiation field in non-LTE, and the emergent spectrum in any case. Therefore, measured values of $b-f$ σ_ν values are very useful. We note that auto-ionizing resonances can greatly complicate the dependence of σ_ν on λ, and cause values computed with simple analytic formulae to be significantly inaccurate (see, for example, Bautista *et al.* (1998)).

Collisional transitions: Cross-sections for excitations and ionizations due to inelastic collisions, mainly with e^-'s and H I, have become increasingly important as a result of the increase in non-LTE modeling. In non-LTE models, the excitation and ionization equilibria of chemical species are calculated by solving a statistical equilibrium among all the processes that populate and de-populate E-levels and ionization states, including *collisional* processes. Therefore, collisional rates have a much more central importance than they do in LTE modeling, and are particularly crucial when collisional transition rates are similar in magnitude to radiative rates. In turn, the calculated opacity, and hence spectral line strength, depends on the computed equilibria. As a result of current uncertainty in collisional σ_ν values, the results of non-LTE modeling must be carefully qualified by laborious perturbation analyses. We note that collisional σ_ν values are needed for dipole-*forbidden* as well as permitted transitions.

Excited states: We note that for realistic modeling, σ_ν values are needed for $b-f$ and collisional transitions arising from *excited* states as well as from the ground state.

3. Special problems requiring improved physical data

3.1. Brown dwarf and Jovian planetary atmospheres

Polyatomic molecular bands: As a result of their low temperatures ($T_{\rm eff} < 3000$ K), brown dwarf atmosphere chemistry admits significant polyatomic molecule formation. Molecular bands that form in the visible and near UV spectral regions (ie. "hot" bands) have a significant effect on both the atmospheric structure and the emergent spectral energy distribution. However, there is a dearth of molecular data for especially important bands of methane (CH_4), water (H_2O), ammonia (NH_3), and iron hydride (FeH). For completely accurate extinction modeling, there is also a need for data for metal hydrides in addition to FeH. See Leggett *et al.* (2001) for examples of observed spectra with molecular bands identified.

With the discovery of an increasing number of extra-solar "hot Jupiter" planets, brown dwarf modeling has been extended downward in temperature to the regime of hot gas giant planets. For these models there is a need for σ_ν values for excitation of H_2 by inelastic collisions.

Atomic resonance line damping: Because the gas pressure in brown dwarf atmospheres is relatively large, the resonance lines of some atomic species, most notably Na I and K I, have Lorentzian damping wings that span over 1000 Å (see Allard *et al.* (2003)). As a result, the wing of a single spectral line acts as a broad-band pseudo-continuous opacity source that significantly affects both the atmospheric structure and the emergent spectral energy distribution. Therefore, it is especially important to accurately model the line profile and to have accurate knowledge of the atomic line broadening parameters.

Aerosols: The low temperatures of brown dwarf atmospheres also allow for the condensation of a large variety of liquid droplet and crystalline grain aerosols. Data is needed for the extinction versus λ for these. Again, their extinction affects both the atmospheric structure and the emergent spectrum (see Allard *et al.* (2003) for example). Important examples for which data is needed are NH_3 and NH_4SH.

3.2. Stars: solar type and cool

CO collisional excitation: The fundamental vibrational ($\Delta\nu = 1$) band of CO at 5μm has been found generally to be stronger than expected in the spectra of solar type and relatively cool stars. The most compelling explanation that has been put forward is that the outer atmospheres of cool stars are thermally bifurcated, with the CO band forming in clouds

of cool gas that are embedded in warmer gas at altitudes that are considered to be purely chromospheric in traditional $1D$ models (Ayres & Wiedemann 1989). If valid, then this interpretation represents a major advance in moving beyond one of the main restrictions of classical stellar spectrum interpretation, namely horizontal homogeneity. However, as noted in Section 2.4, the true excitation equilibrium of a chemical species may depend on collisional transition rates. Therefore, the correct interpretation of the strength of the $\Delta\nu = 1$ band depends on the adopted value of σ_ν for the excitation of CO by inelastic collisions with H I. Currently, these σ_ν values are estimated by scaling σ_ν values for collisional excitation by H_2, and are uncertain by a factor of approximately 100. The large uncertainty limits the ability to model the atmospheric structure on the basis of the $\Delta\nu = 1$ band with certainty.

SiO collisional excitation: Similarly, more accurate knowledge of the σ_ν value for collisional excitation by H I of SiO would be helpful for modeling maser emission in the vicinity of very large cool stars. Masing occurs in an extreme non-LTE equilibrium, thus collisional transition rates are important.

Silicate dust in winds: In cool stars with dusty winds the measured density of silicate dust grains is greater than expected on the basis of the gas density in the wind. One explanation is that the physical data relevant to silicate grain nucleation and condensation is inadequate. Silicate grain formation has not been as well studied as that of carbon grains.

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